

Pentachloroethane
76-01-7 | DTXSID7021104

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 39.2

Global applicability domain: Inside

Local applicability domain index: 6.32e-01

Confidence level: 6.74e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,1,2,2-Tetrachloroethane</div> <div>Measured: 12.9</div> <div>Predicted: 11.4</div>	<div>Image not found</div> <div>Tetrachloroethylene</div> <div>Measured: 52.5</div> <div>Predicted: 42.2</div>	<div>Image not found</div> <div>Hexachloroethane</div> <div>Measured: 513</div> <div>Predicted: 452</div>
<div>Image not found</div> <div>Carbon tetrachloride</div> <div>Measured: 7.41</div> <div>Predicted: 12.9</div>	<div>Image not found</div> <div>1,2,2,3-Tetrachloropropane</div> <div>Measured: 37.2</div> <div>Predicted: 20.8</div>	